

Mechanism of Fermi Level Pinning at Metal/Germanium Interfaces

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The physical origin of Fermi level pinning (FLP) at metal/Ge interfaces has been argued over a long period. Using the Fe₃Si/Ge(111) heterostructure developed originally, we can explore electrical transport properties through atomically matched metal/Ge junctions. Unlike the conventional metal/*p*-Ge junctions reported so far, we clearly observe rectifying current-voltage characteristics with a measurable Schottky barrier height, depending on the contact area of the Fe₃Si/Ge(111) junction. These results indicate that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will be developed for understanding FLP for almost all the metal/semiconductor interfaces.

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The fundamental mechanism of the formation of the Schottky barrier at metal/semiconductor interfaces has so far been studied over a long period.[1–9] In particular, the controversy about the physical origin of Fermi level pinning (FLP) at the metal/semiconductor interfaces remains unsolved.[10] In order to interpret FLP, the metal-induced gap states (MIGS),[1, 6] caused by the decay of traveling wave function from the metal electrode into the band gap of the semiconductor, have been suggested. The MIGS are considered to be intrinsic mechanisms. In contrast, other extrinsic mechanisms such as defect-induced gap states at the interface have been discussed.[3, 5, 8]

Development of high mobility germanium (Ge) based metal-oxide-semiconductor field effect transistors (MOSFETs) is required for breaking down the ultimate scaling limit of silicon (Si)-based conventional complementary metal-oxide-semiconductor transistors.[11] However, FLP is one of the critical issues even at metal/Ge interfaces,[10] disturbing the development of high-performance MOSFETs with metallic source and drain contacts. In general, the influence of FLP on metal/Ge interfaces is stronger than that on metal/Si ones. The strong FLP always results in relatively high Schottky barrier height (SBH: $\Phi_b \sim 0.6$ eV) for metal/*n*-Ge junctions and ohmic characteristics for metal/*p*-Ge ones, arising from the charge neutrality level close to the valence band edge of Ge.[12, 13]

Recently, effective alleviation of the strong FLP was also demonstrated by an insertion of ultra-thin insulating layers between a metal and Ge,[14, 15] in which electrical properties of the metal/*n*-Ge and metal/*p*-Ge junctions were varied to ohmic and rectifying characteristics with increasing the thickness of the insertion layer. It seems that the observed thickness dependence is strongly related to the blocking of the penetration of the wave

function of electrons in the band gap of Ge. Thus, one has believed that the strong FLP at metal/Ge interfaces is predominantly due to MIGS,[14–16] i.e., intrinsic mechanisms. On the other hand, several groups have discussed the influence of extrinsic mechanisms such as dangling bonds on the strong FLP.[17–21] Therefore, exploring the mechanism of FLP at metal/Ge interfaces is not only important for demonstrating high-performance MOSFETs but also for understanding FLP for almost all the metal/semiconductor interfaces.

In order to elucidate the origin of the strong FLP, we propose that the use of the high-quality Fe₃Si(111)/Ge(111) junction with an atomically matched interface is effective.[20] Fe₃Si has a Heusler-type crystal structure[22, 23] and there is almost no lattice mismatch between Fe₃Si (0.564 ~ 0.566 nm) and Ge (0.565 nm). Furthermore, the atomic matching at the junction between Fe₃Si(111) and Ge(111) is theoretically perfect, as illustrated in Fig. 1 of Ref.[20]. To date, we clarified that, for Fe₃Si/*n*-Ge(111) junctions, the SBH is unexpectedly lower ($\Phi_b \sim 0.46$ eV) than that due to the strong FLP reported so far (0.55 ~ 0.65 eV) and, for Fe₃Si/*p*-Ge(111) junctions, rectifying behavior in current-voltage (*I*-*V*) characteristics is seen below 170 K.[20] Though these results have implied the presence of an extrinsic mechanism of the strong FLP, we have not yet obtained its reliable evidence. At least, we should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces.

In this Letter, we experimentally study the mechanism of the strong FLP at metal/Ge interfaces using the atomically matched Fe₃Si/Ge(111) heterostructure. For the high-quality Fe₃Si/*p*-Ge(111) junctions, we can easily observe the clear Schottky characteristics with a measurable Schottky barrier height, depending on the contact area of the Fe₃Si/Ge(111) junction. These transport data can be understood by the model based on the influence of the interfacial defects such as dangling bonds, and indicate that one should distinguish between intrinsic and

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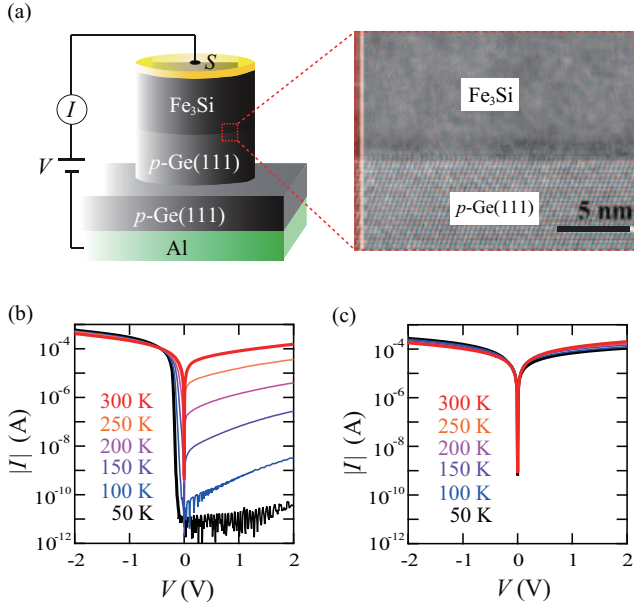


FIG. 1: (Color online) (a) The schematic illustration of the fabricated junctions with various areas (S). The enlarged picture is a cross-sectional transmission electron micrograph of the atomically controlled Fe₃Si/Ge(111) interface. (b), (c) I - V characteristics of representative two junctions with $S = \sim 1 \mu\text{m}^2$. (b) Marked rectifying and (c) ohmic behavior with the temperature evolution.

extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will be developed for understanding FLP for almost all the metal/semiconductor interfaces.

Prior to the fabrication of the Fe₃Si/Ge(111) heterostructure, p -Ge(111) substrates were chemically cleaned to remove contamination and native oxide from the surface, where the p -Ge(111) substrates were already on the market ($p = 9 \times 10^{14} \text{ cm}^{-3}$). The cleaned substrates were loaded immediately into an ultra high vacuum chamber with a base pressure of $\sim 10^{-7} \text{ Pa}$. After the surface heat treatment conducted at 550 °C for 20 min, the substrate temperature was reduced down to 200°C. An atomically clean surface was confirmed by observing the reflection high-energy electron diffraction (RHEED) patterns. Using low-temperature molecular beam epitaxy (MBE),[24] we grew the epitaxial Fe₃Si layer with a thickness of 50 nm on p -Ge(111). During the growth, two-dimensional epitaxial growth was confirmed by the observation of RHEED patterns. After the growth, we fabricated Schottky diodes with a contact area S ($S = \sim 1, \sim 10^2$, and $\sim 10^6 \mu\text{m}^2$) to examine electrical properties of the Fe₃Si/ p -Ge(111) junctions.[20] Here all the diodes used in this study were fabricated from one Fe₃Si/ p -Ge(111) wafer. The schematic diagram of the fabricated Fe₃Si/ p -Ge/Al Schottky junctions is shown in Fig. 1(a), where a backside Al is an Ohmic contact. The Fe₃Si/Ge(111) interface is atomically flat,[20, 24] as shown in a cross-sectional transmis-

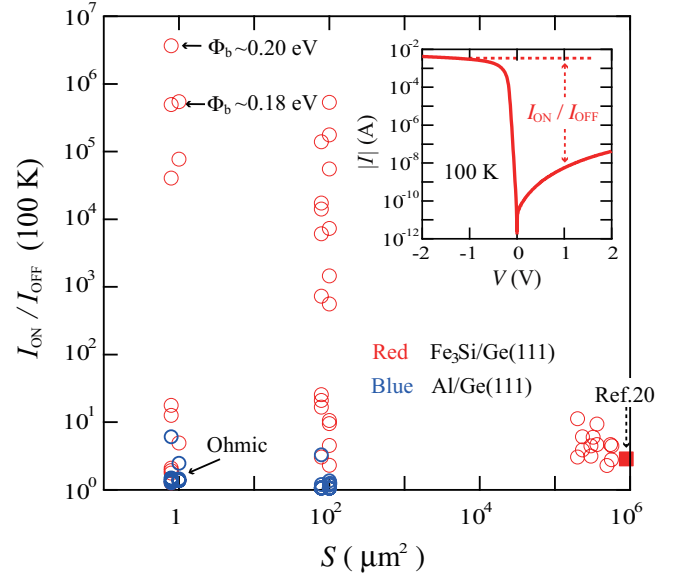


FIG. 2: (Color online) Summary of $I_{\text{ON}}/I_{\text{OFF}}$ ratio measured at 100 K for various Fe₃Si/ p -Ge(111)/Al junctions (red) with $S = \sim 1, \sim 10^2$, and $\sim 10^6 \mu\text{m}^2$, together with that for Al/ p -Ge(111)/Al (blue) junctions. The red-square symbol at $\sim 10^6 \mu\text{m}^2$ is the data for a sample shown in Ref. [20]. The inset shows an I - V characteristic for a junction with $S = \sim 10^2 \mu\text{m}^2$ at 100 K. The $I_{\text{ON}}/I_{\text{OFF}}$ ratio is defined at $V = \pm 1 \text{ V}$.

sion electron micrograph (TEM) image in Fig. 1(a). To compare the atomically matched high-quality junctions with other mismatched ones, we also fabricated Al/ p -Ge(111) junctions with the atomically mismatched interface by using the same MBE equipment after the same surface cleaning. The growth temperature of the Al/ p -Ge(111) junctions was less than 25 °C.

First of all, we have studied I - V characteristics for lots of Fe₃Si/ p -Ge(111) junctions with $S = \sim 1 \mu\text{m}^2$. Figures 1(b) and 1(c) show representative I - V characteristics at various temperatures. Despite the directly connected metal/Ge structure, we observe marked rectifying behavior in Fig. 1(b) at low temperatures surprisingly. The ratio of the forward current (I_{ON}) to the reverse current (I_{OFF}) reaches $\sim 10^8$ at 50 K. The reverse bias current ($V > 0$) increases with increasing temperature, implying the presence of an evident Schottky barrier. A rectifying I - V characteristic can be obtained even at 300 K. Using the thermionic emission theory,[25] we can roughly obtain Φ_b for hole transport. From the I - T characteristics,[20] the Φ_b for holes in Fig. 1(b) was estimated to be $\sim 0.18 \text{ eV}$, which is the first experimental observation of Φ_b in the directly connected metal/ p -Ge junctions. In contrast, almost ohmic characteristics are seen in Fig. 1(c) even at low temperatures, consistent with the strong FLP.[12, 13] This means that the tunneling conduction occurs through the very low and thin Schottky barrier. When we decreased temperature from 50 to 10 K, we observed very small rectifications in I - V characteristics. Note that despite almost the same de-

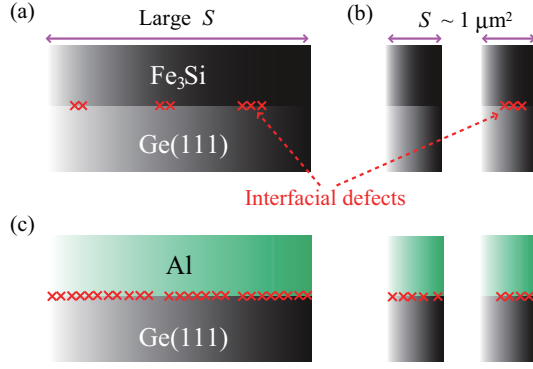


FIG. 3: (Color online) The schematic diagrams of the model for the $\text{Fe}_3\text{Si}/\text{Ge}(111)$ interface with (a) large S and (b) small S . There are some interfacial defects even at the atomically matched interface. (c) The diagrams in the case of the atomically mismatched $\text{Al}/\text{Ge}(111)$ interface.

vices fabricated from the same wafer there are different I - V characteristics for $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions with $S = \sim 1 \mu\text{m}^2$. We also measured the I - V characteristics of the $\text{Al}/p\text{-Ge}(111)$ junctions with $S = \sim 1 \mu\text{m}^2$, measured at various temperatures, and then, almost all the junctions showed ohmic I - V characteristics, also consistent with the strong FLP.[12, 13] For the $\text{Al}/p\text{-Ge}(111)$ junctions, we sometimes observed very small rectifications in I - V characteristics as the temperature was decreased down to 10 K. However, we could not estimate Φ_b for $\text{Al}/p\text{-Ge}(111)$. We emphasize that clear Schottky characteristics were achieved only when we used the atomically matched $\text{Fe}_3\text{Si}/\text{Ge}(111)$ interface.

To understand the interesting features described above, we further examined the effect of S on I - V characteristics for many junctions in detail. As a consequence, we easily observed rectifying behavior in the I - V curves at low temperatures for many $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions. In Fig. 2 we summarize $I_{\text{ON}}/I_{\text{OFF}}$ at 100 K for various $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions with $S = \sim 1$, $\sim 10^2$, and $\sim 10^6 \mu\text{m}^2$, together with the data for $\text{Al}/p\text{-Ge}(111)$ junctions. Here for all kinds of S we measured I - V curves of more than fifteen junctions, and the $I_{\text{ON}}/I_{\text{OFF}}$ values were roughly defined as the data at $V = \pm 1$ V, as shown in the inset. In the main figure we can reconfirm that, for the $\text{Al}/p\text{-Ge}(111)$ junctions with the atomically mismatched interfaces, all the $I_{\text{ON}}/I_{\text{OFF}}$ values are less than 10^1 even for the smallest junctions with $S = \sim 1 \mu\text{m}^2$, consistent with the strong FLP. On the other hand, for the $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions, we can evidently see the difference in the $I_{\text{ON}}/I_{\text{OFF}}$ values depending strongly on S . For the large junctions ($S = \sim 10^6 \mu\text{m}^2$), the $I_{\text{ON}}/I_{\text{OFF}}$ values are almost constant ($\sim 10^1$). The small rectification of the I - V curves disappeared at ~ 170 K, similar to our previous work.[20] In contrast, for the small junctions with $S = \sim 1$ and $\sim 10^2 \mu\text{m}^2$, the $I_{\text{ON}}/I_{\text{OFF}}$ values are scattered from the wide range $10^0 \leq I_{\text{ON}}/I_{\text{OFF}} \leq 10^7$. For $S = \sim 1 \mu\text{m}^2$ the junctions shown in Figs. 1(b) and 1(c), i.e., $\Phi_b \sim 0.18$ eV and ohmic, respectively, are also plotted in

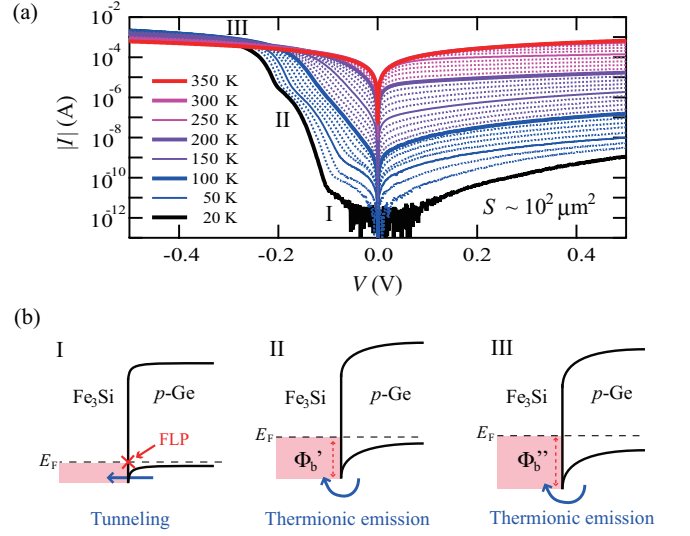


FIG. 4: (Color online) (a) Temperature evolution of I - V characteristics with three-step staircase in forward bias ($V < 0$), observed in $\text{Fe}_3\text{Si}/\text{Ge}(111)$ junctions with $S = \sim 10^2 \mu\text{m}^2$. (b) Schematic illustrations of the hole transport in $V < 0$ at low temperatures. There are plural current channels in the $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions and all the channels contribute to the forward-bias current.

Fig. 2 (see arrows), and the junction with $\Phi_b \sim 0.20$ eV shows the largest $I_{\text{ON}}/I_{\text{OFF}} \sim 7 \times 10^6$. The scattering of the $I_{\text{ON}}/I_{\text{OFF}}$ values in Fig. 2 implies that many kinds of the Schottky barriers are distributed for our $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions. We discuss it later. Note that the scattering range for $S = \sim 1 \mu\text{m}^2$ is narrow ($I_{\text{ON}}/I_{\text{OFF}} < \sim 10^1$, $\sim 10^5 < I_{\text{ON}}/I_{\text{OFF}} < 10^7$) compared to $S = \sim 10^2 \mu\text{m}^2$ ($I_{\text{ON}}/I_{\text{OFF}} < \sim 10^2$, $10^3 < I_{\text{ON}}/I_{\text{OFF}} < 10^6$).

Hereafter we intensively discuss the effect of S on $I_{\text{ON}}/I_{\text{OFF}}$, presented in Fig. 2. For almost all the $\text{Al}/p\text{-Ge}(111)$ junctions, we can regard the small $I_{\text{ON}}/I_{\text{OFF}}$ values of $\sim 10^0$ at low temperatures as consequences of the strong influence of FLP on the hole transport. In short, there is almost no effect of S on $I_{\text{ON}}/I_{\text{OFF}}$ at low temperatures. On the other hand, there is the marked effect of S on $I_{\text{ON}}/I_{\text{OFF}}$ for the $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ junctions. Even if we use the atomically matched $\text{Fe}_3\text{Si}(111)/\text{Ge}(111)$ junctions shown in Fig. 1 of Ref. [20], there will be still some atomic imperfection at the (111) planes between Fe or Si in Fe_3Si and Ge, giving rise to the defects such as dangling bonds in Ge at the interface. Therefore, the presence of some unintentional defects at the $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$ interface can be considered generally. Assuming Poisson distribution for the defects at the $\text{Fe}_3\text{Si}/\text{Ge}(111)$ interface, we can show a possible scenario considering the correlation between S and interfacial defects as follows. When S is large such as $S = \sim 10^6 \mu\text{m}^2$, the $\text{Fe}_3\text{Si}/\text{Ge}(111)$ junction includes the some interfacial defects, as schematically illustrated in Fig. 3(a). The observed small $I_{\text{ON}}/I_{\text{OFF}}$ values of $\sim 10^1$ in Fig. 2 should be regarded as consequences of the influence of the inter-

facial defects on hole transport properties. On the other hand, when we reduce S as small as possible, we can encounter the two different interfaces, as shown in Fig. 3(b). Then, we can obtain almost no or a strong contribution of the defects to the transport properties. Surely, for $S = \sim 1 \mu\text{m}^2$, we have already obtained such two different contributions in Figs. 1(b) and (c). Also, we can regard the two discrete regions in Fig. 2, i.e., $I_{\text{ON}}/I_{\text{OFF}} < \sim 10^1$ and $\sim 10^5 < I_{\text{ON}}/I_{\text{OFF}} < 10^7$, as the above two different contributions. In contrast, since there are a large number of interfacial defects at the atomically mismatched Al/ p -Ge(111) interfaces, as illustrated in Fig. 3(c), we cannot encounter the situation with almost no interfacial defect even if we use the small junctions which we can fabricate. Since we have not obtained the data with Schottky characteristics even for the smallest Al/ p -Ge(111) junctions, the above scenario based on the influence of the interfacial defects on the hole transport can also be applied to the atomically mismatched interfaces.

Recent papers also indicated that passivation techniques of the Ge surface can work effectively for changing electrical properties of the metal/Ge junctions.[18, 19, 21] Also, theoretical studies suggested that the defect levels lie just above the valence band,[26, 27] indicating that the previous experimental results shown in Ref. [12, 13] originate from the interfacial defects such as dangling bonds. These studies strongly support our new findings in this paper. We want to emphasize that lots of researchers have so far observed the predominant influence of interfacial defects on the transport properties of metal/Ge junctions. In other words, this study indicates that if one discusses the fundamental mechanism of the formation of the Schottky barrier at metal/Ge interfaces, one should consider the influence of interfacial defects, i.e., extrinsic mechanisms. In the future, we will need further exploration of the method for reducing the number of the defects formed at the atomically matched metal/Ge interfaces.

Finally, we discuss the scattering of the $I_{\text{ON}}/I_{\text{OFF}}$ values in Fig. 2 for $S = \sim 1$ and $\sim 10^2 \mu\text{m}^2$. For $S = \sim 1 \mu\text{m}^2$, the various Fe₃Si/ p -Ge(111) interfaces with Schottky barriers from $\Phi_b \sim 0.20$ eV to almost ohmic were demonstrated. Also, the scattering range for $S = \sim 1 \mu\text{m}^2$ is narrower than that for $S = \sim 10^2 \mu\text{m}^2$. This feature indicates that the scattering of the $I_{\text{ON}}/I_{\text{OFF}}$ values is related to S , i.e., the number of interfacial defects. Since the $I_{\text{ON}}/I_{\text{OFF}}$ value is usually attributed to Φ_b , we should interpret that Φ_b is also related to the number of defects. Thus, somewhat different contributions of the number of defects to Φ_b can be considered in the Fe₃Si/Ge(111) junctions. On the basis of

this consideration, we show new findings for electrical properties in the Fe₃Si/Ge(111) junctions. Figure 4(a) displays the I - V curves for an Fe₃Si/ p -Ge(111) junction with $S = \sim 10^2 \mu\text{m}^2$ at various temperatures. Interestingly, we can see the staircase-like I - V characteristics in forward bias ($V < 0$), denoted by I, II, and III. In this study, we frequently observed these staircase-like I - V characteristics for $S = \sim 10^2 \mu\text{m}^2$ at low temperatures though the room-temperature I - V curves were almost the same ohmic characteristics. The interpretation of the staircase-like I - V characteristics is shown in Fig. 4(b). That is, there are plural current channels for holes, resulting from the tunneling conduction due to FLP (I) and from the thermionic-emission conduction (II, III) with two different Schottky barriers with Φ_b' and Φ_b'' . At low temperatures the forward bias current ($V < 0$) can detect the contributions of all the current channels, while, with increasing temperature, Φ_b' and Φ_b'' cannot affect the transport properties, giving rise to the disappearance of the staircase-like behavior. This feature means that there are different contributions of the interfacial defects to Φ_b for just one Fe₃Si/ p -Ge(111) interface in the middle-sized junctions. By using the atomically matched Fe₃Si/ p -Ge(111) interface, we can evidently observe some new findings for electrical properties of metal/Ge interfaces. This study indicates that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces.

In summary, we have studied the mechanism of FLP at metal/Ge junctions using the atomically matched Fe₃Si/Ge(111) interface. Despite metal/ p -Ge interfaces, we clearly observed rectifying current-voltage characteristics with a measurable Schottky barrier height, depending on the contact area of the Fe₃Si/Ge(111) junction. These data can be understood by the model based on the influence of the interfacial defects such as dangling bonds, and indicate that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will give us an important principle for understanding FLP for almost all the metal/semiconductor interfaces, which has been studied over a long period.

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